

Supplementary Material

A Convenient and Efficient Synthesis of 3-benzofuryl-substituted phthalides

Yongjun Zang,^a Qilin Xu,^a Guosi Li,^a Shaoshuai Bi,^a YunFeng Ma,^{b*} and Fucheng Zhu^{a*}

^a*Traditional Chinese Medicine Institute of Anhui Dabie Mountain, Department of Biological and Pharmaceutical Engineering, West Anhui University, Lu'an, Anhui 237012, P.R. China.*

^b*Anhui Anlito Biological Technology Co., LTD, Anhui Huoshan Economic and Technological Development Zone 237200, P.R. China*

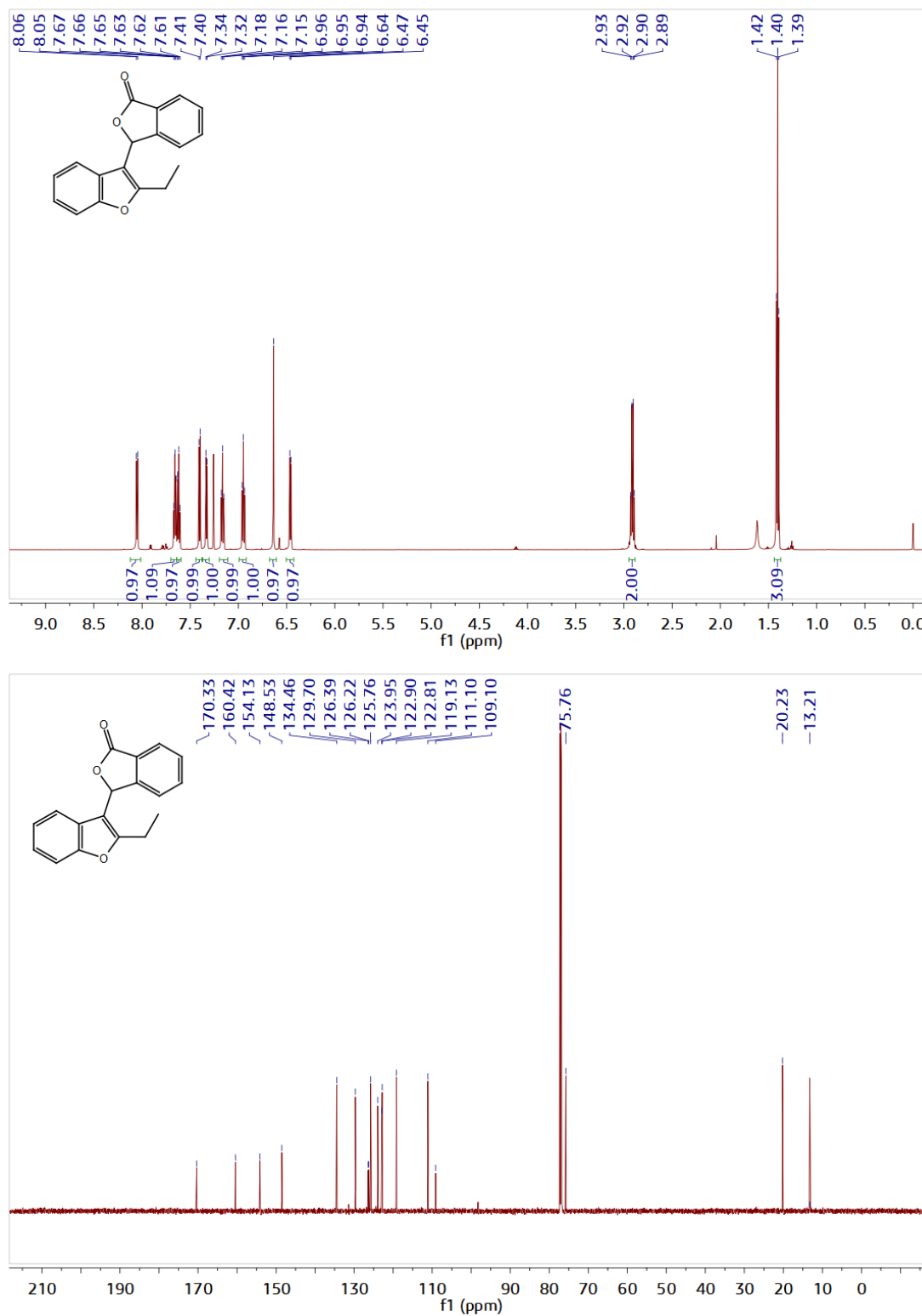
E-mail: 1973636151@qq.com and fucheng323@163.com

Table of Contents

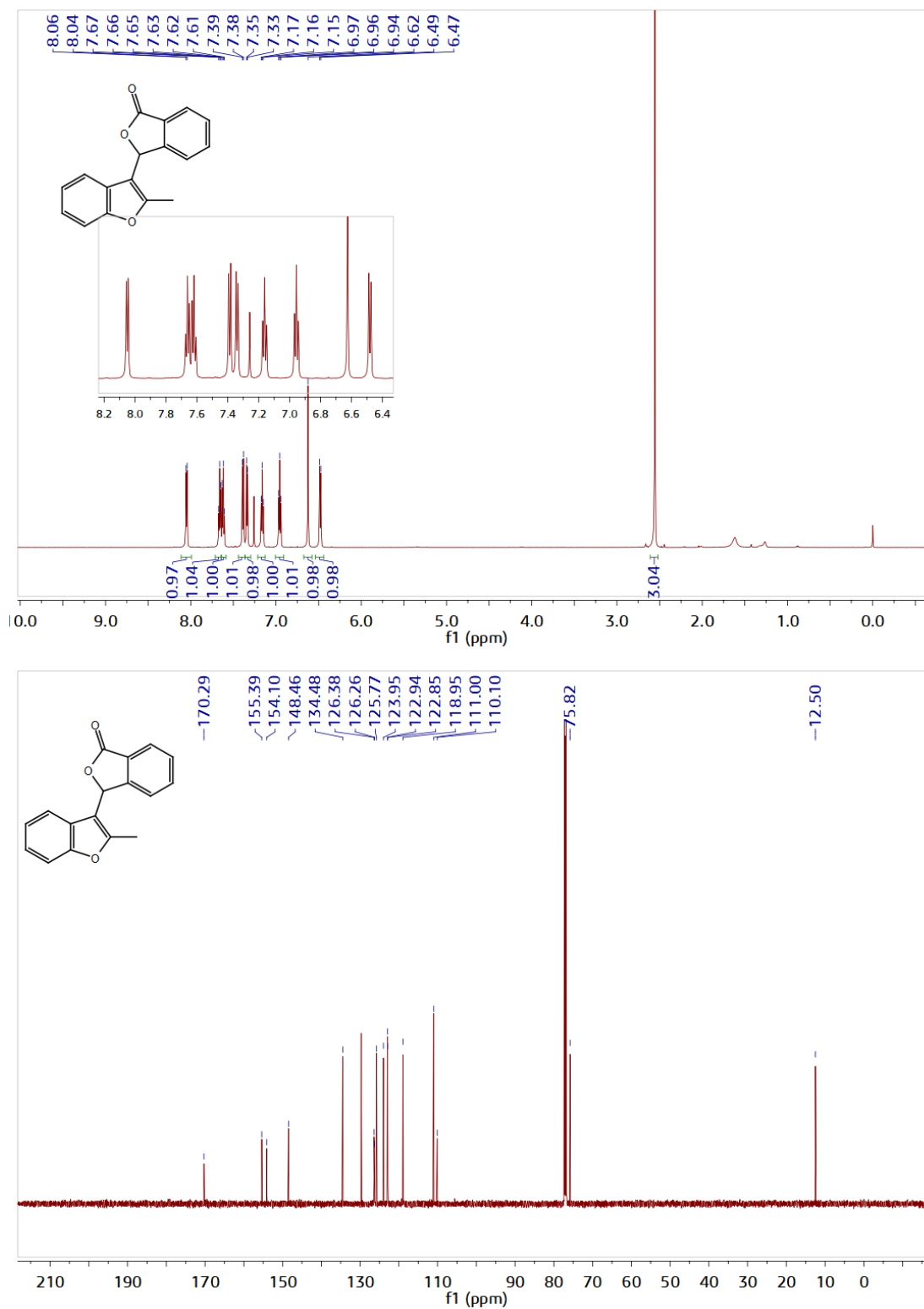
1. ¹ H NMR and ¹³ C NMR Spectra.....	S2
2. X-ray crystallographic data for 3e	S23

1. ^1H NMR and ^{13}C NMR Spectra

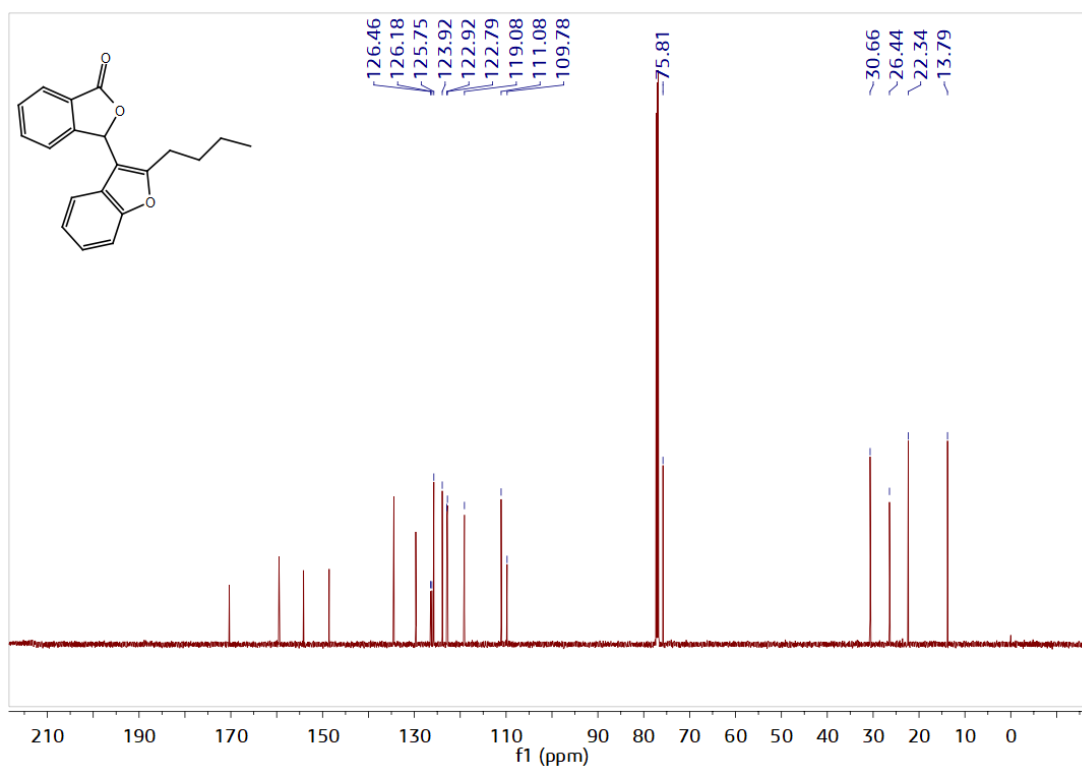
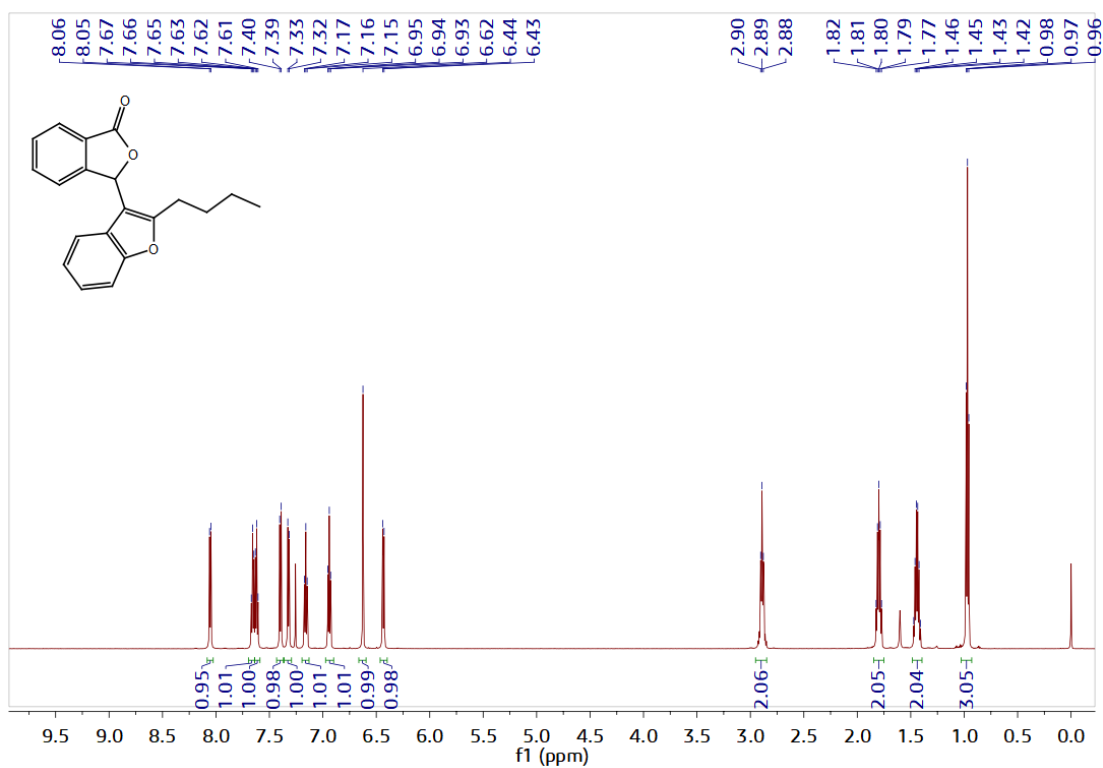
3-(2-ethylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3a). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



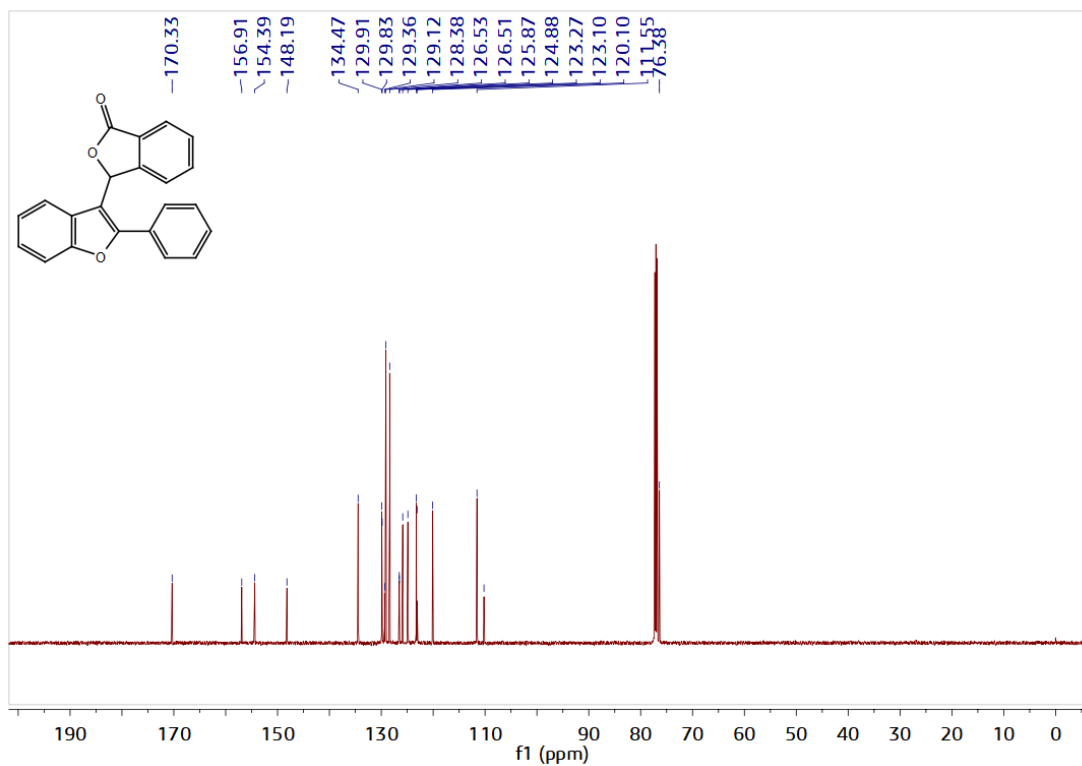
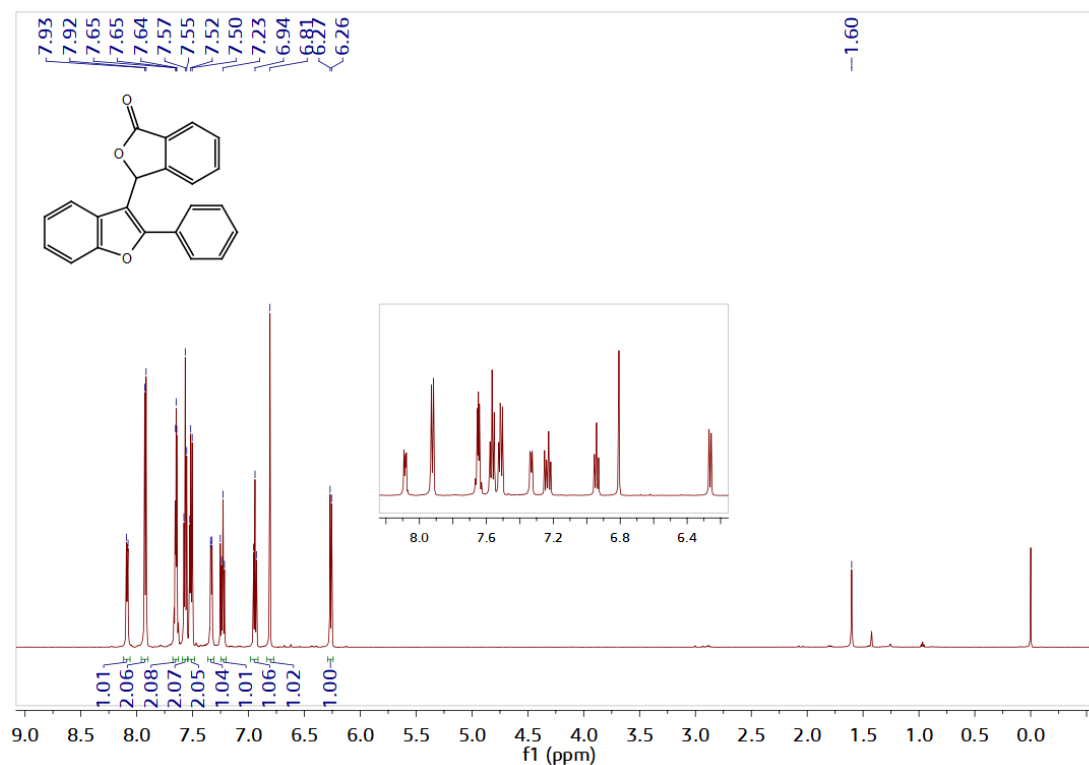
3-(2-methylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3b). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

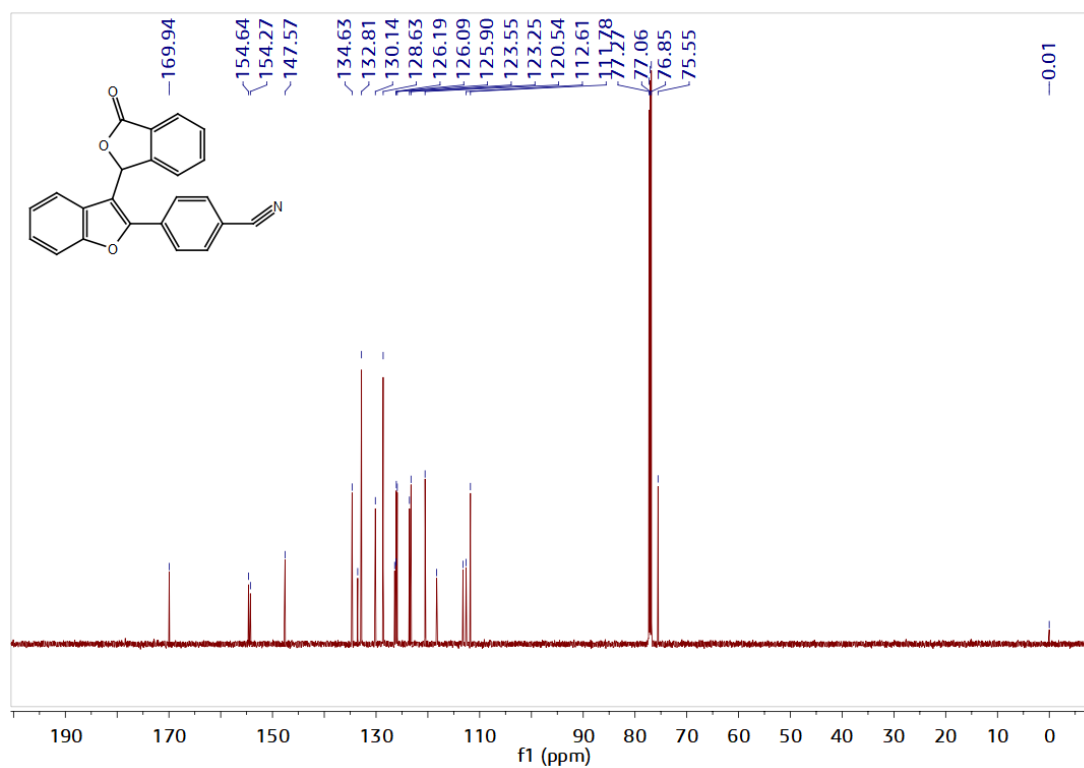
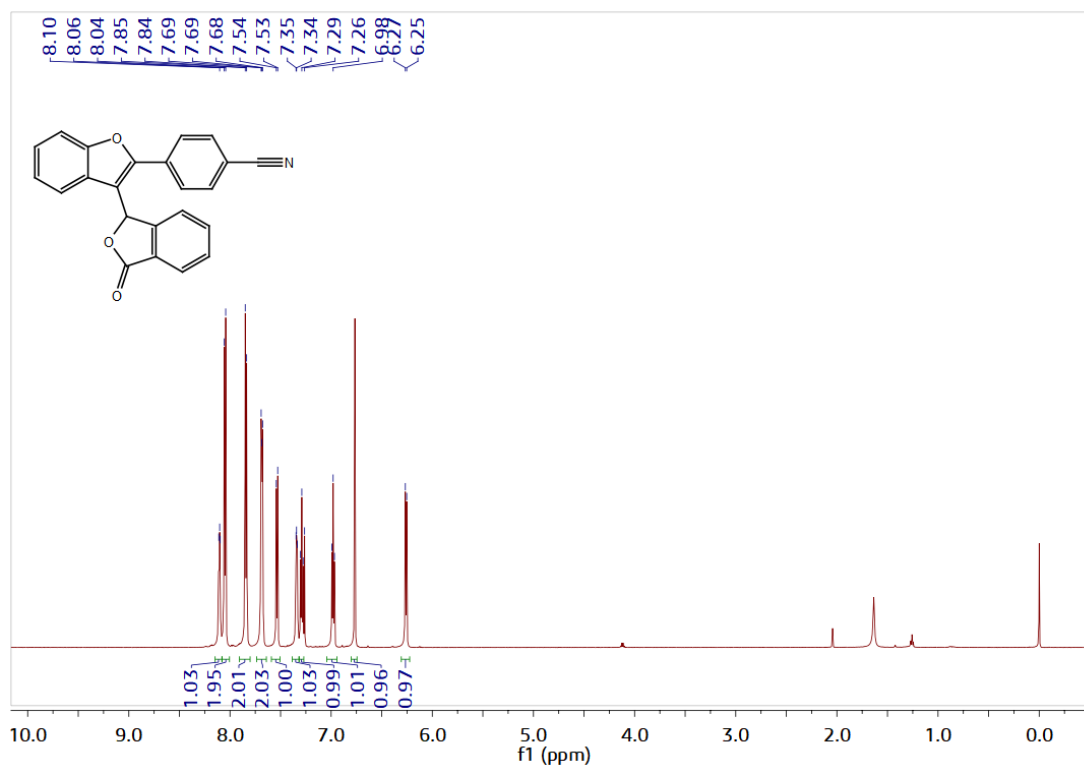


3-(2-butylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3c). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

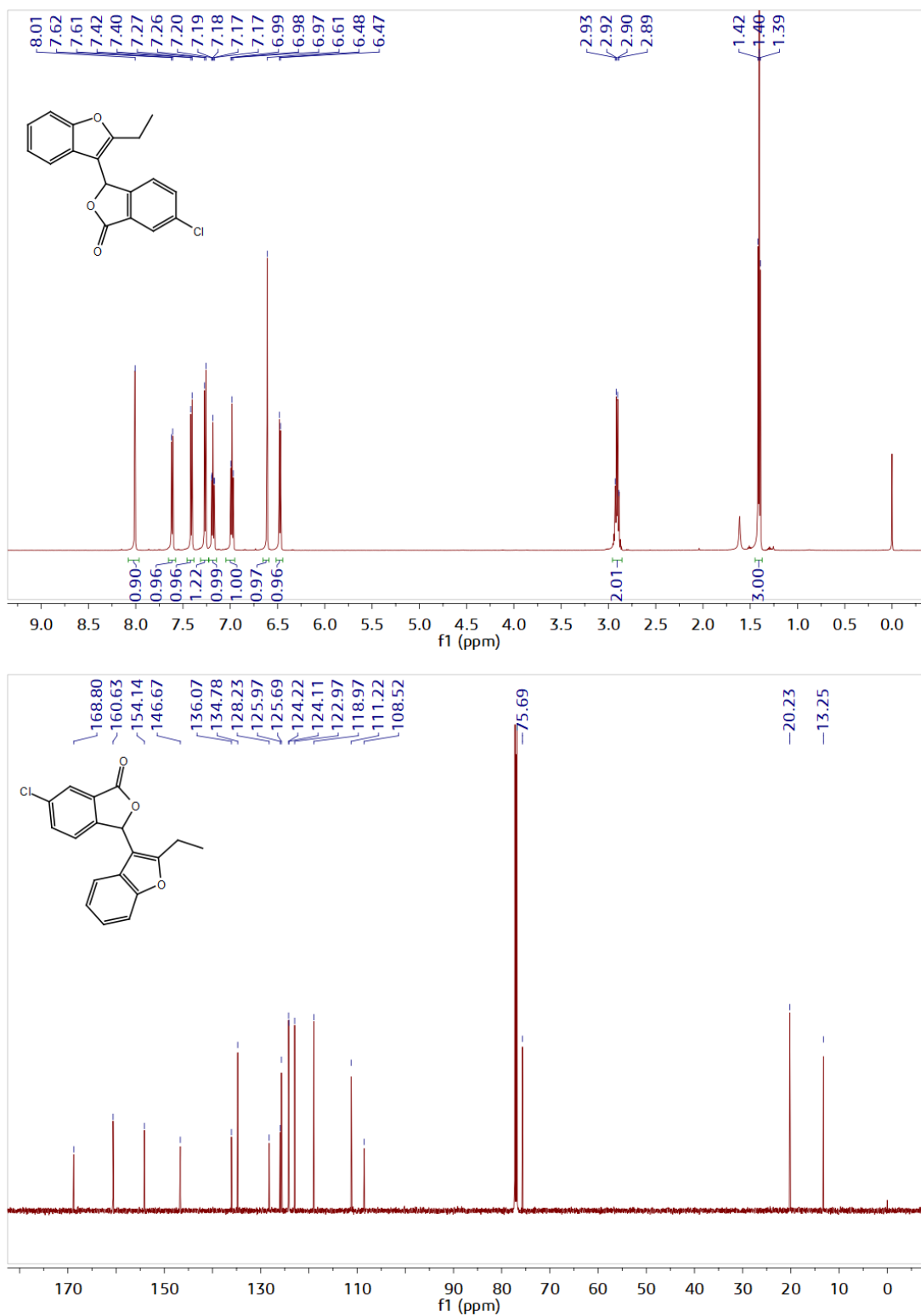


3-(2-phenylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3d). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

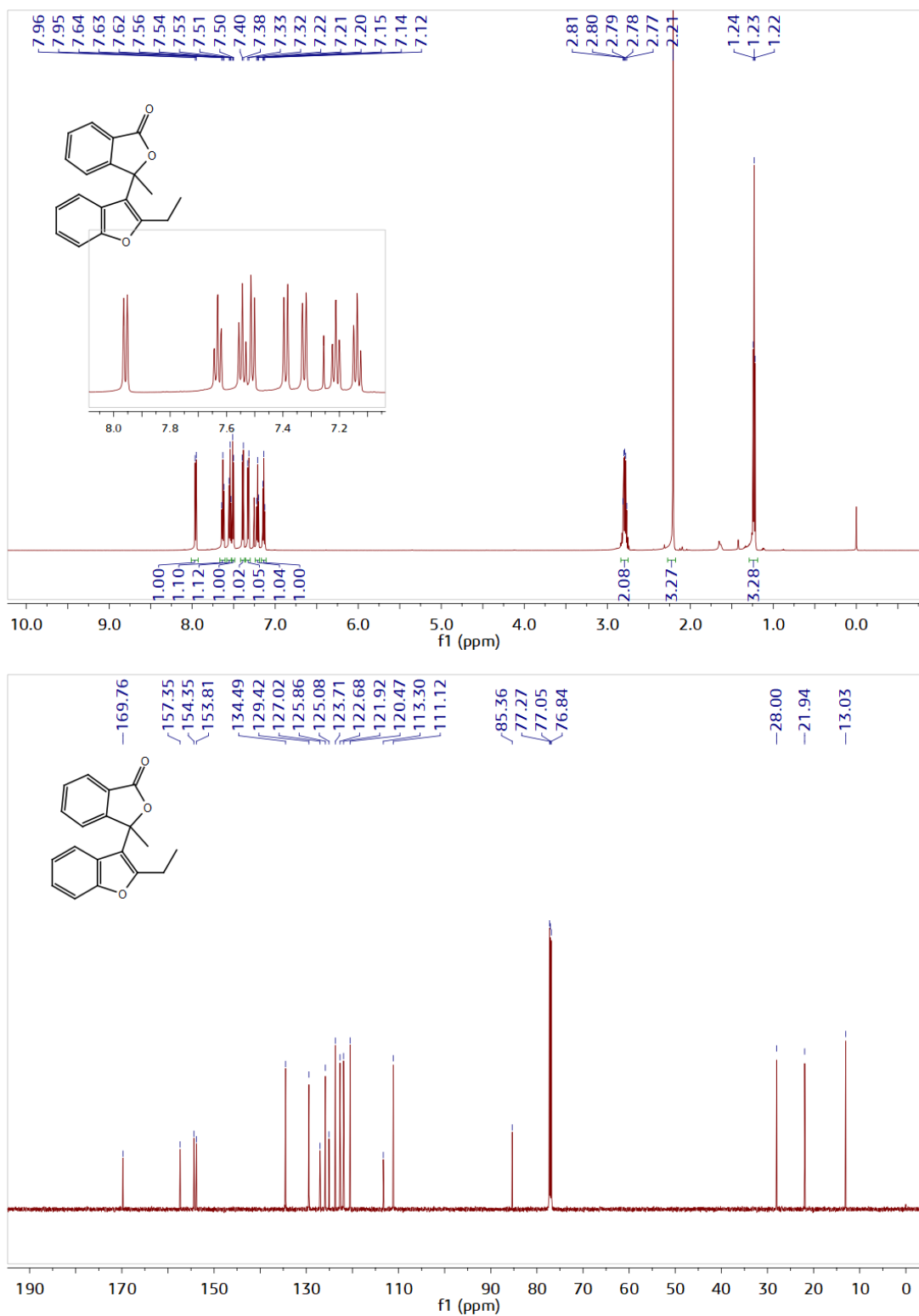


4-(3-(3-oxo-1,3-dihydroisobenzofuran-1-yl)benzofuran-2-yl)benzonitrile (3e).¹H NMR (600 MHz, CDCl₃); ¹³C NMR (151 MHz, CDCl₃)

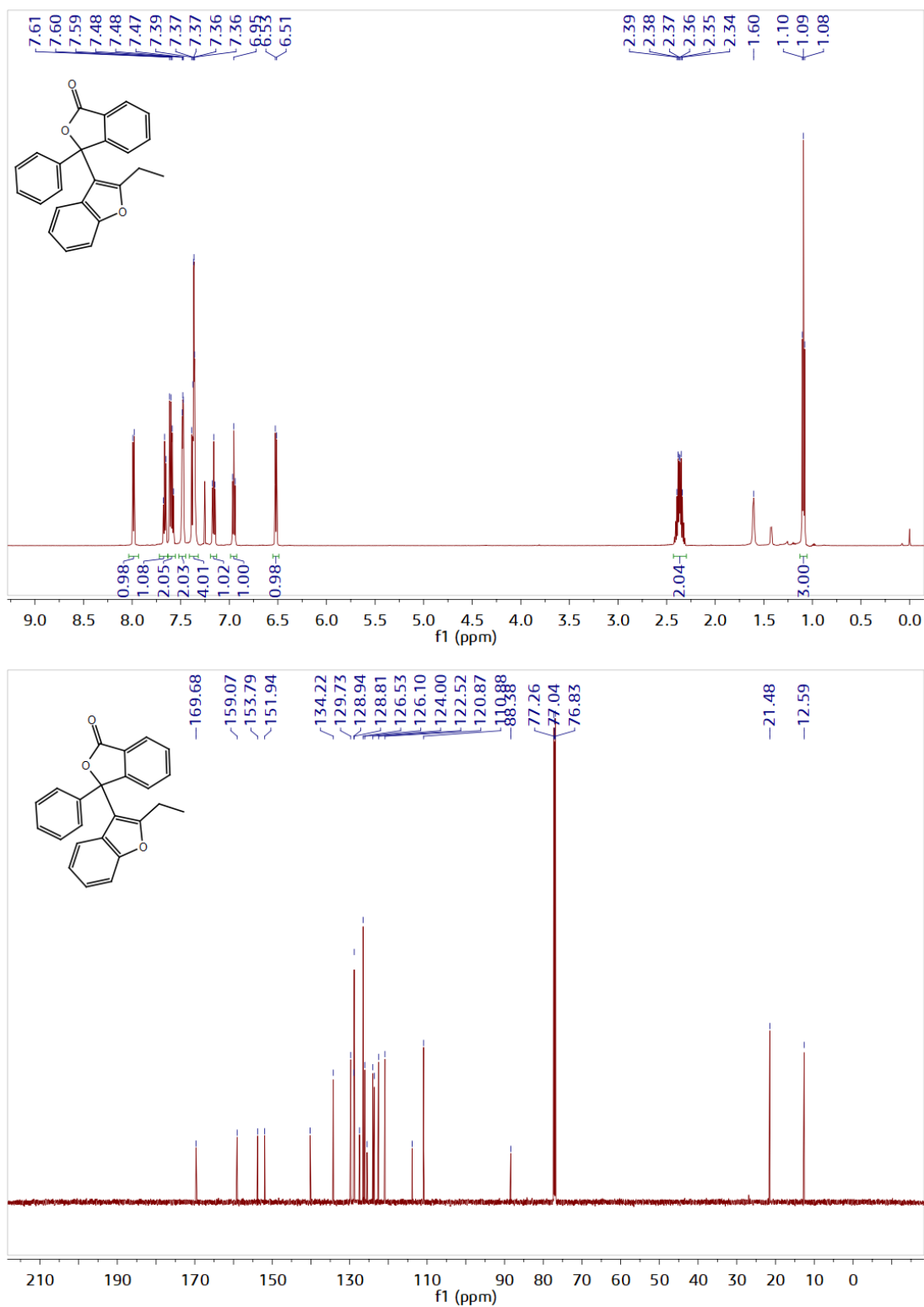
6-chloro-3-(2-ethylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3f). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



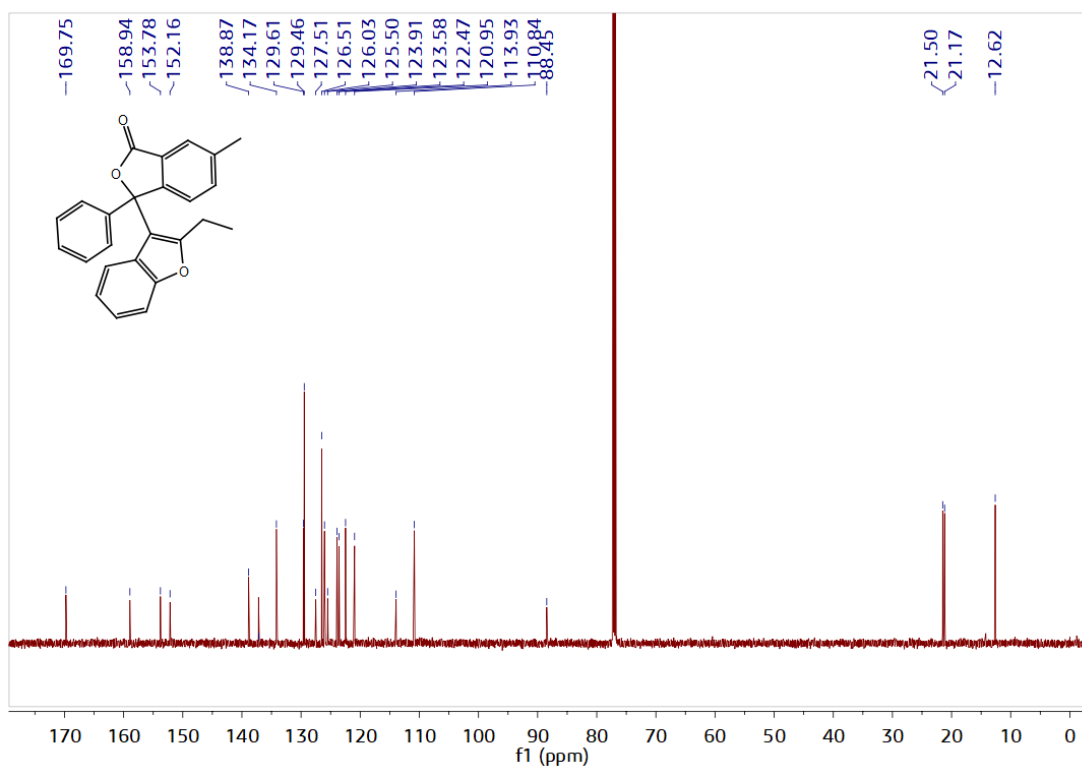
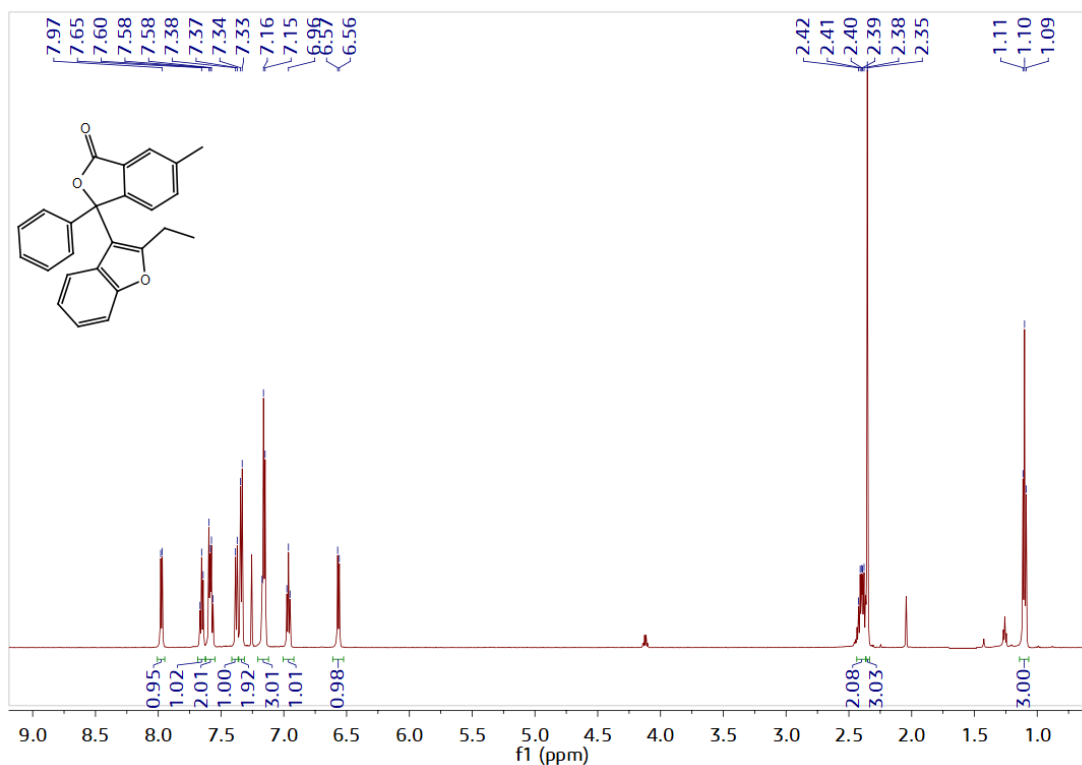
3-(2-ethylbenzofuran-3-yl)-3-methylisobenzofuran-1(3H)-one (3h). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



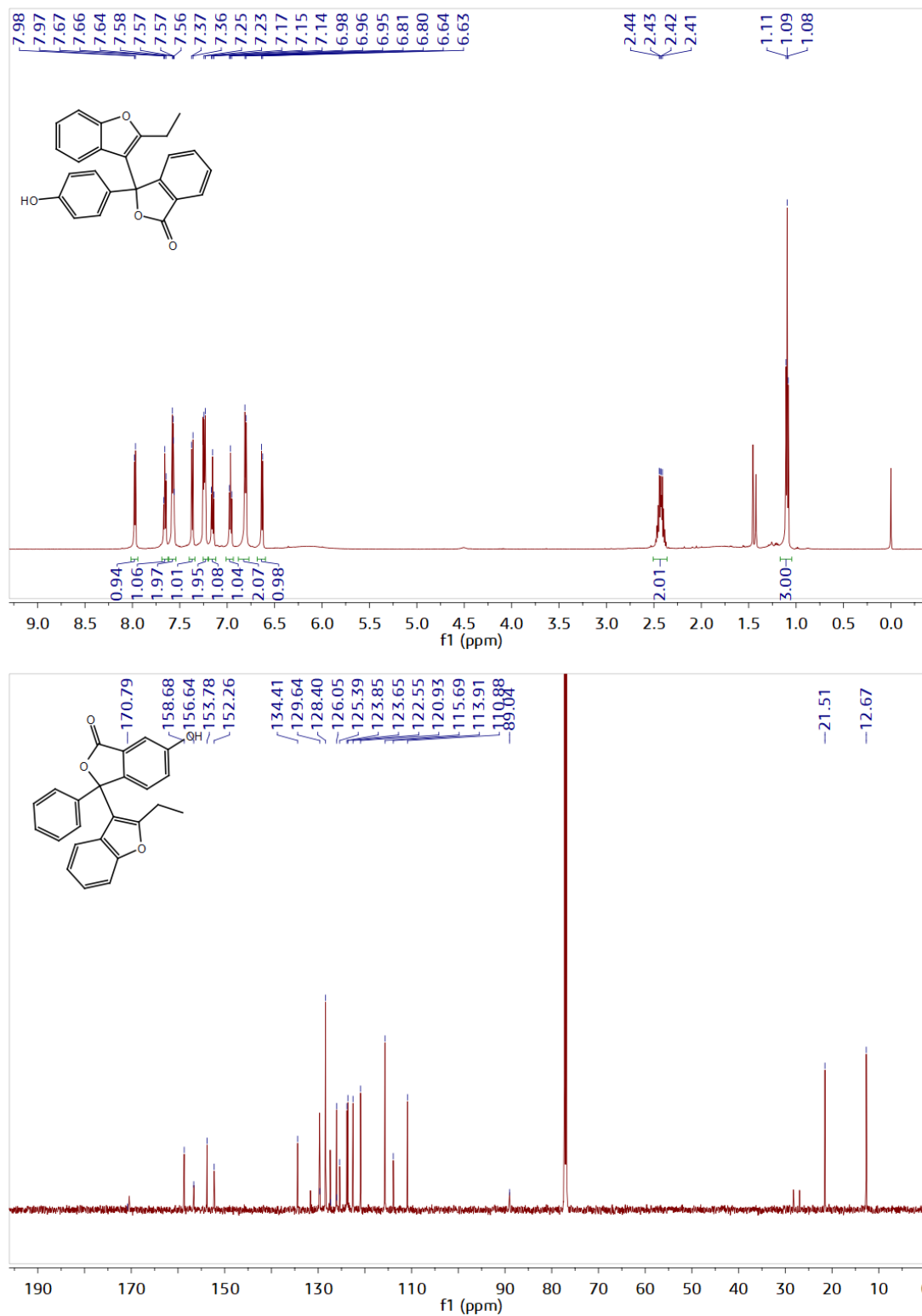
3-(2-ethylbenzofuran-3-yl)-3-phenylisobenzofuran-1(3H)-one (3i). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



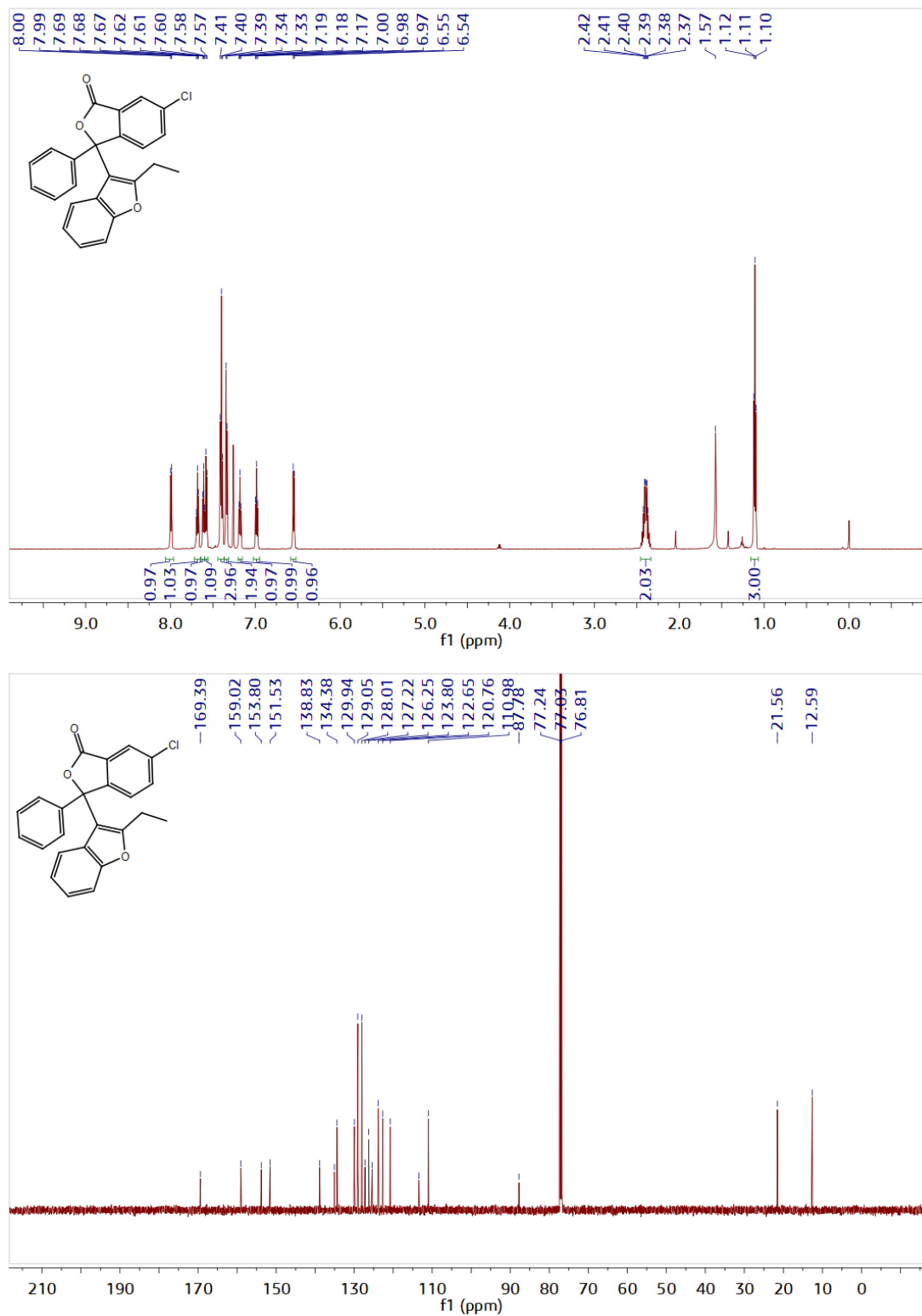
3-(2-ethylbenzofuran-3-yl)-6-methyl-3-phenylisobenzofuran-1(3H)-one (3j). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



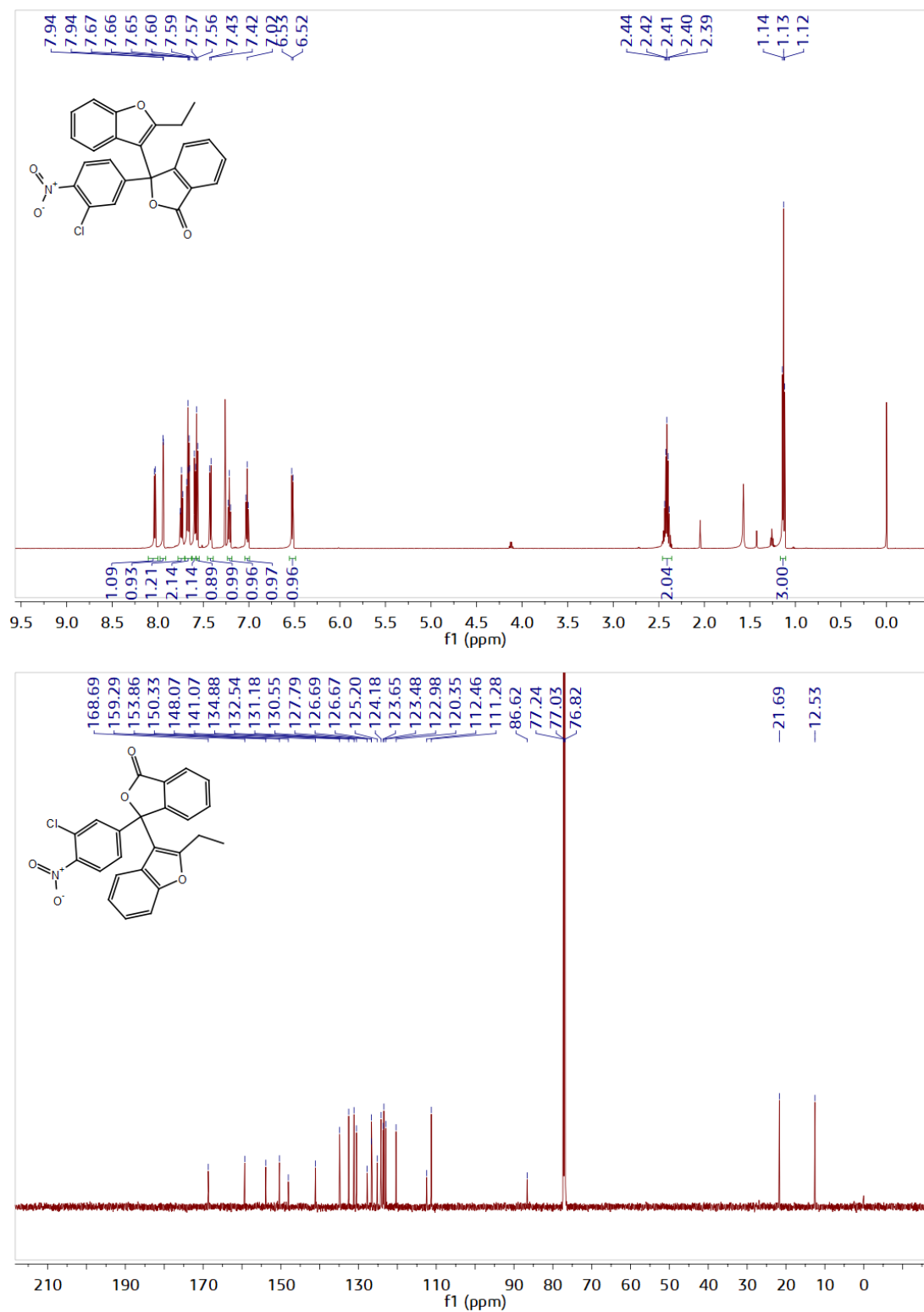
3-(2-ethylbenzofuran-3-yl)-6-hydroxy-3-phenylisobenzofuran-1(3H)-one (3k). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



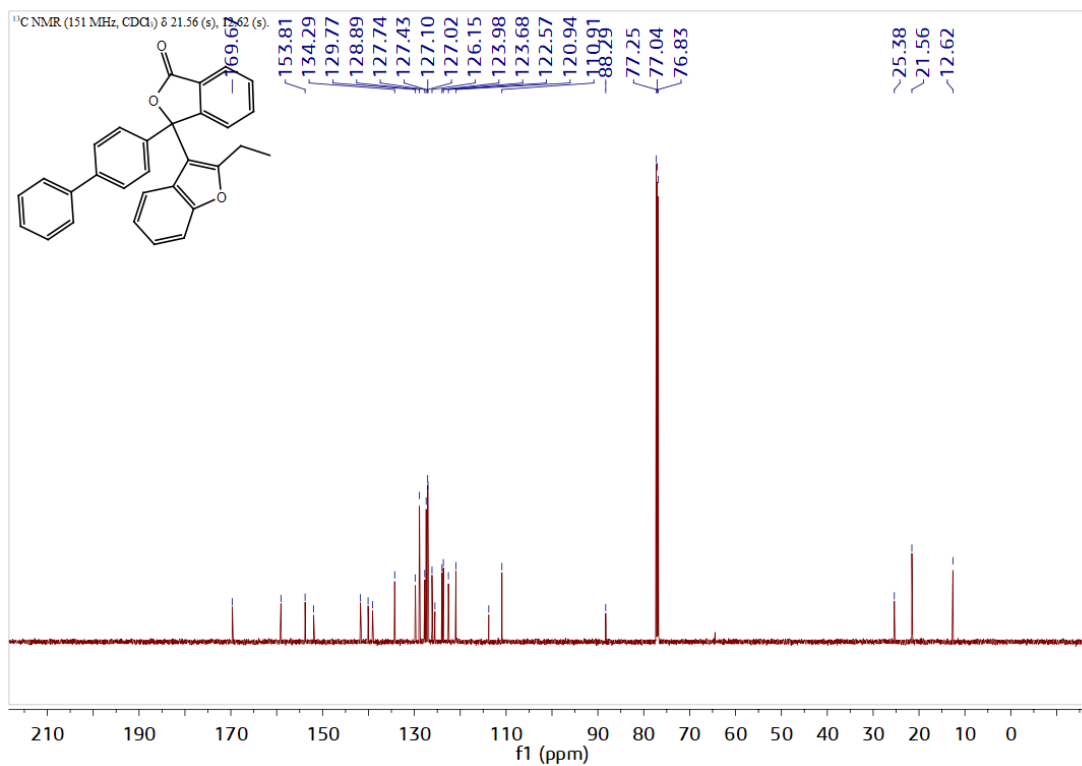
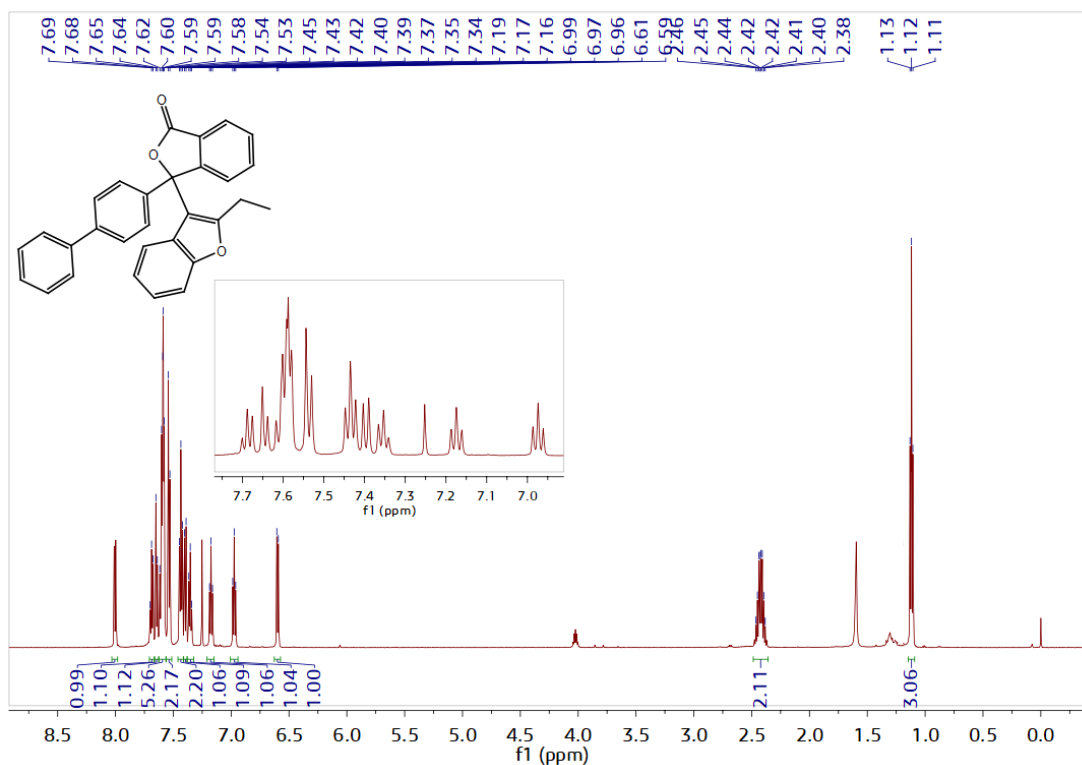
6-chloro-3-(2-ethylbenzofuran-3-yl)-3-phenylisobenzofuran-1(3H)-one (3I). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



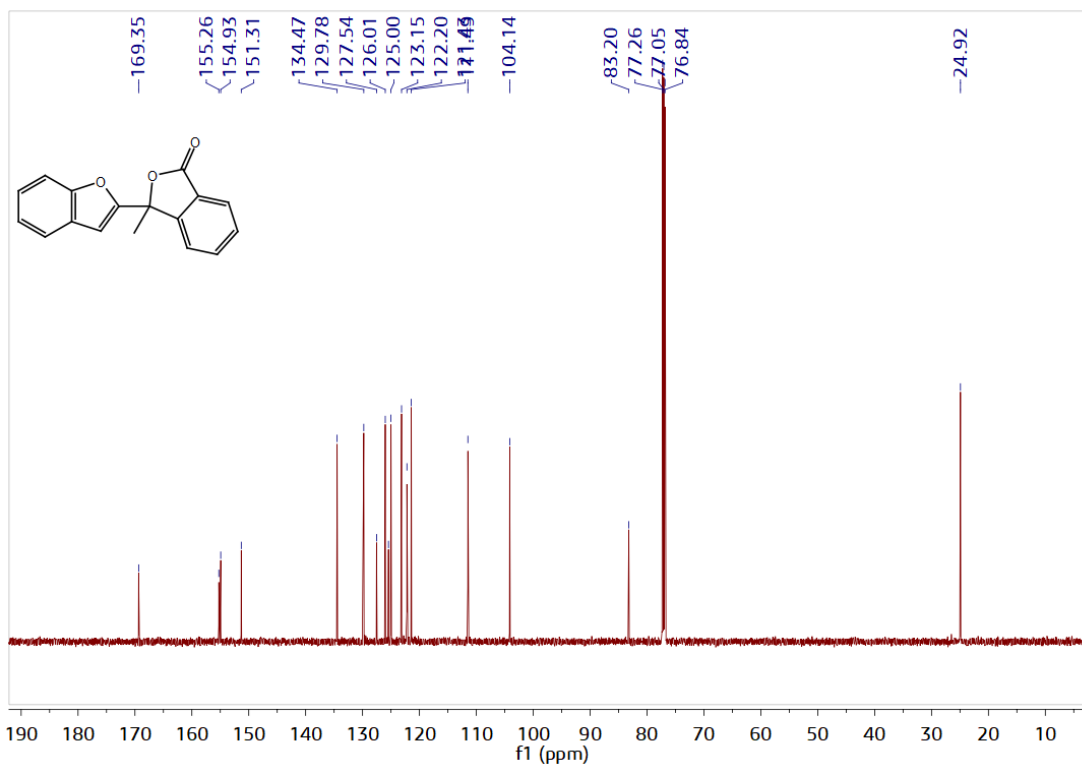
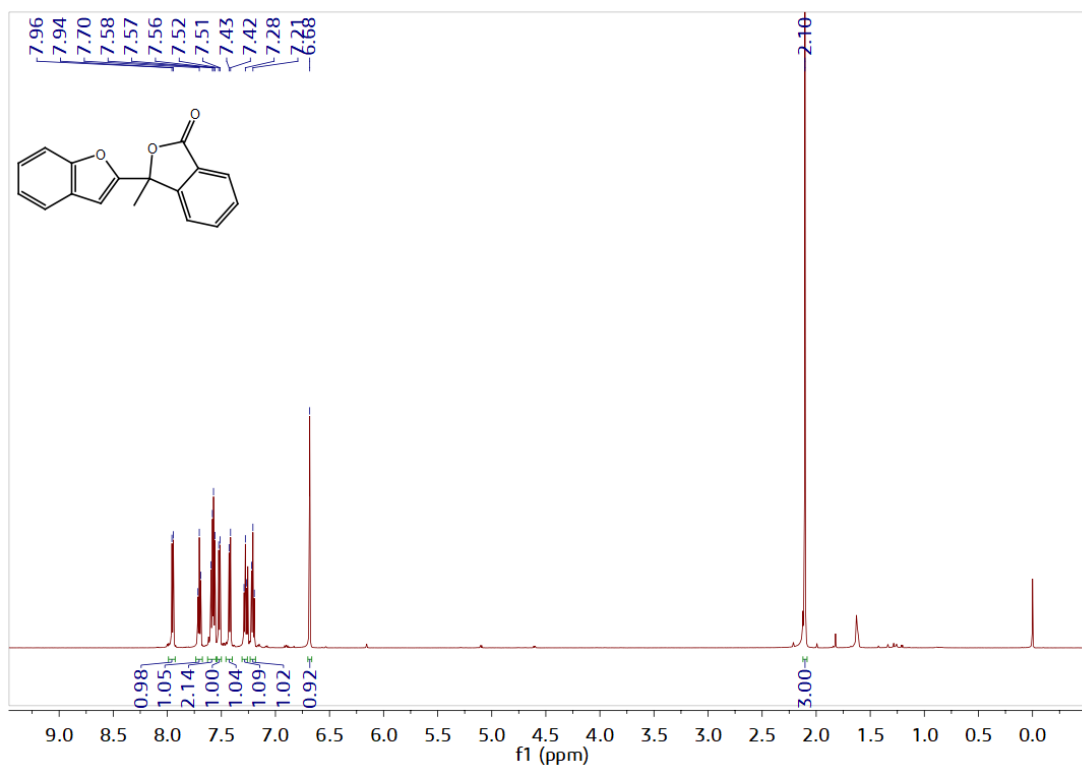
3-(3-chloro-4-nitrophenyl)-3-(2-ethylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3m). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



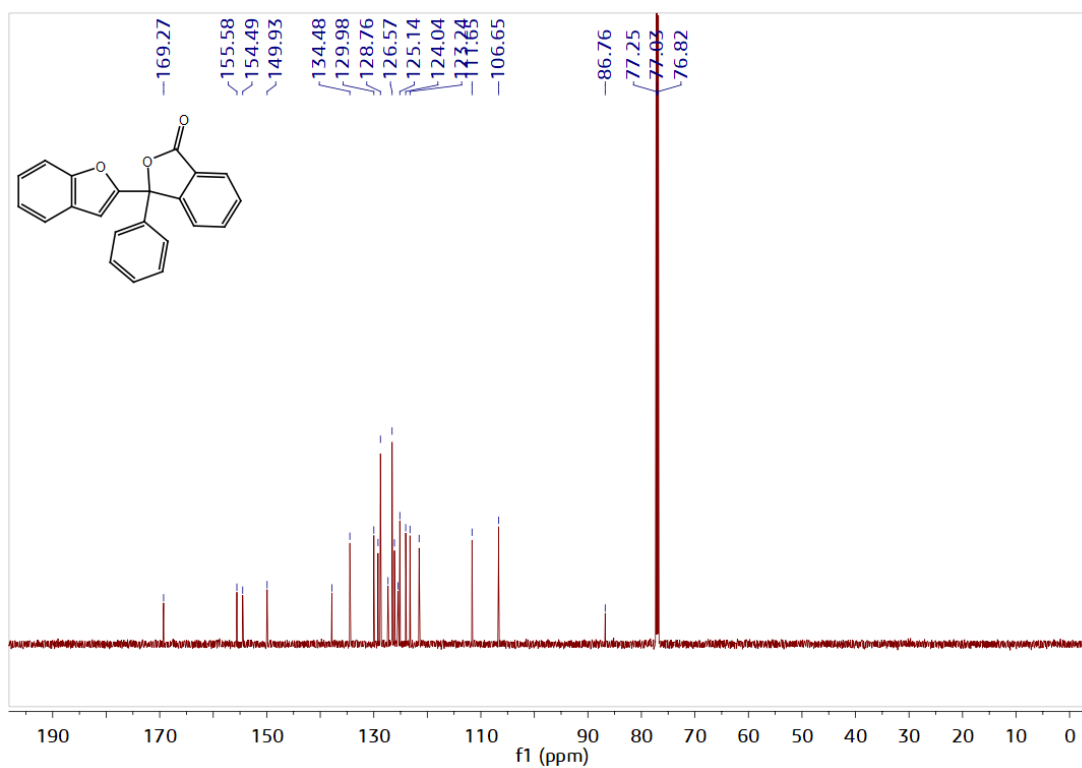
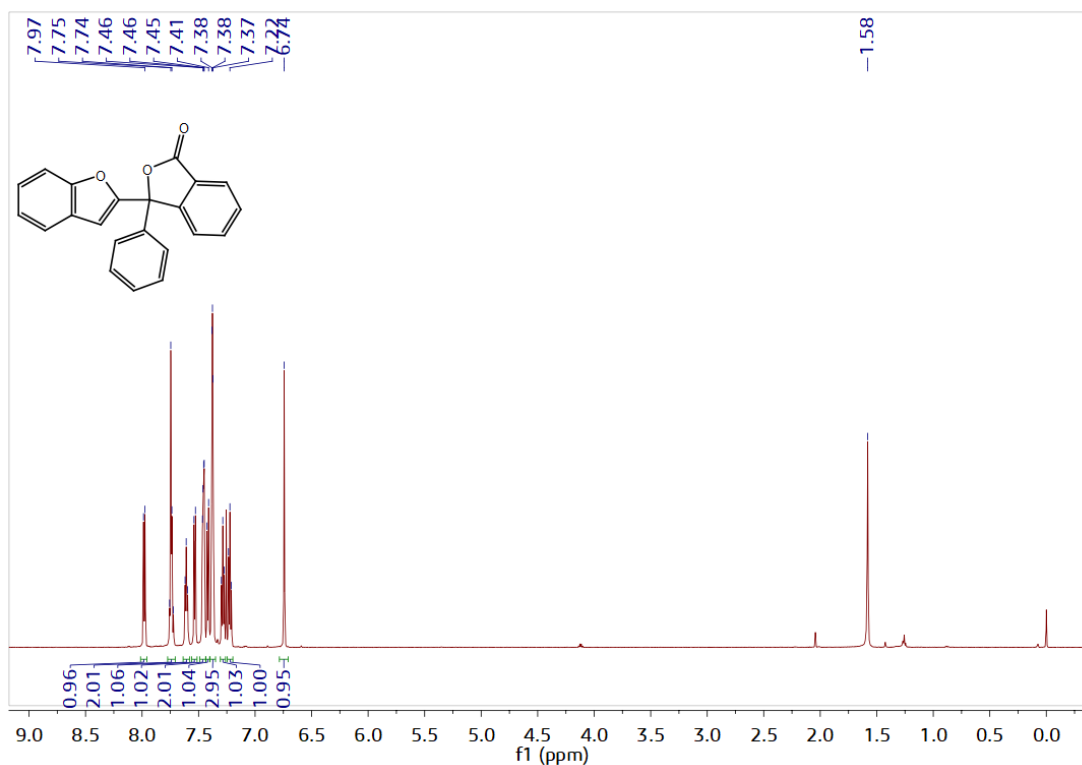
3-([1,1'-biphenyl]-4-yl)-3-(2-ethylbenzofuran-3-yl)isobenzofuran-1(3H)-one (3n). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



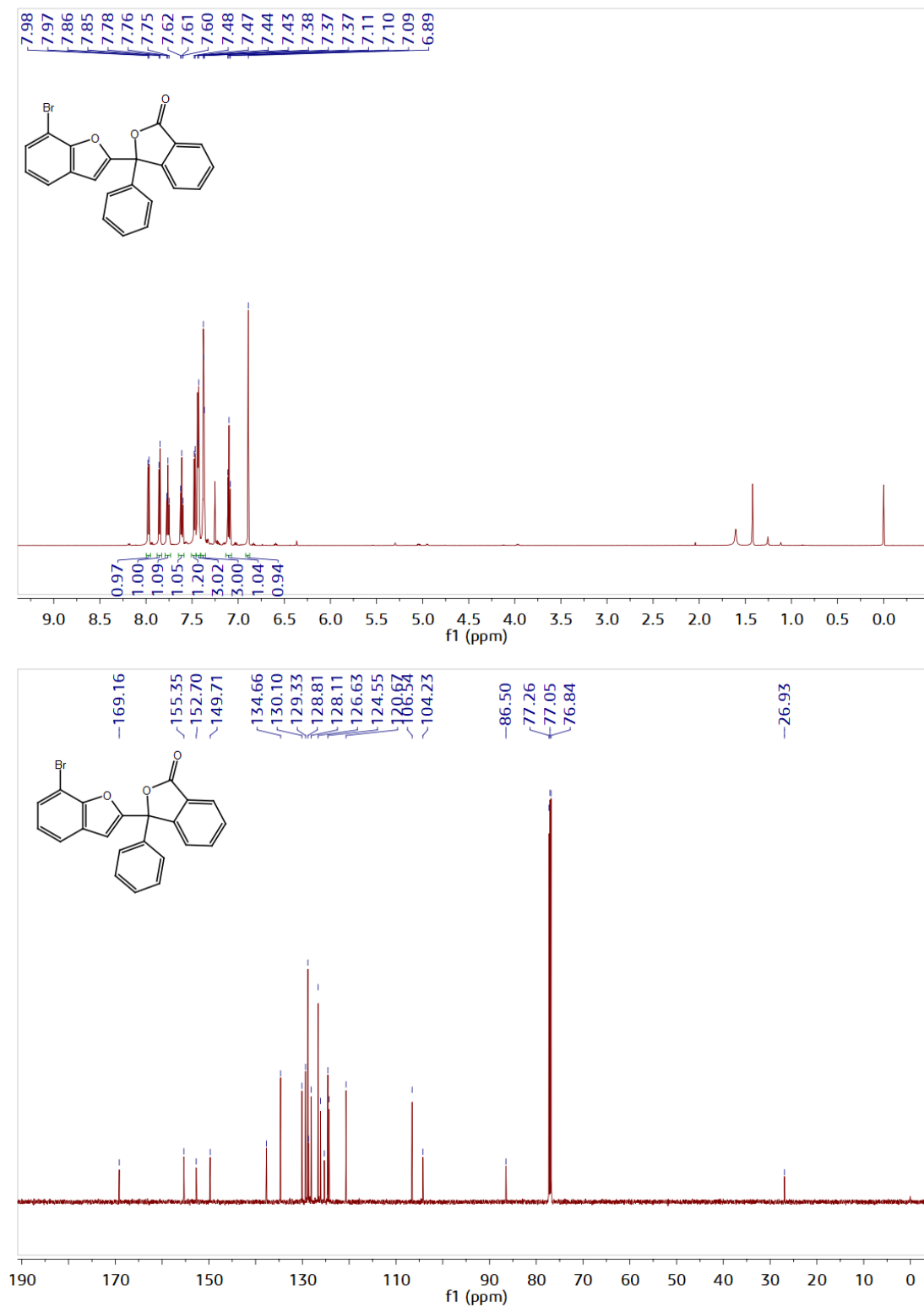
3-(benzofuran-2-yl)-3-methylisobenzofuran-1(3H)-one (3o). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



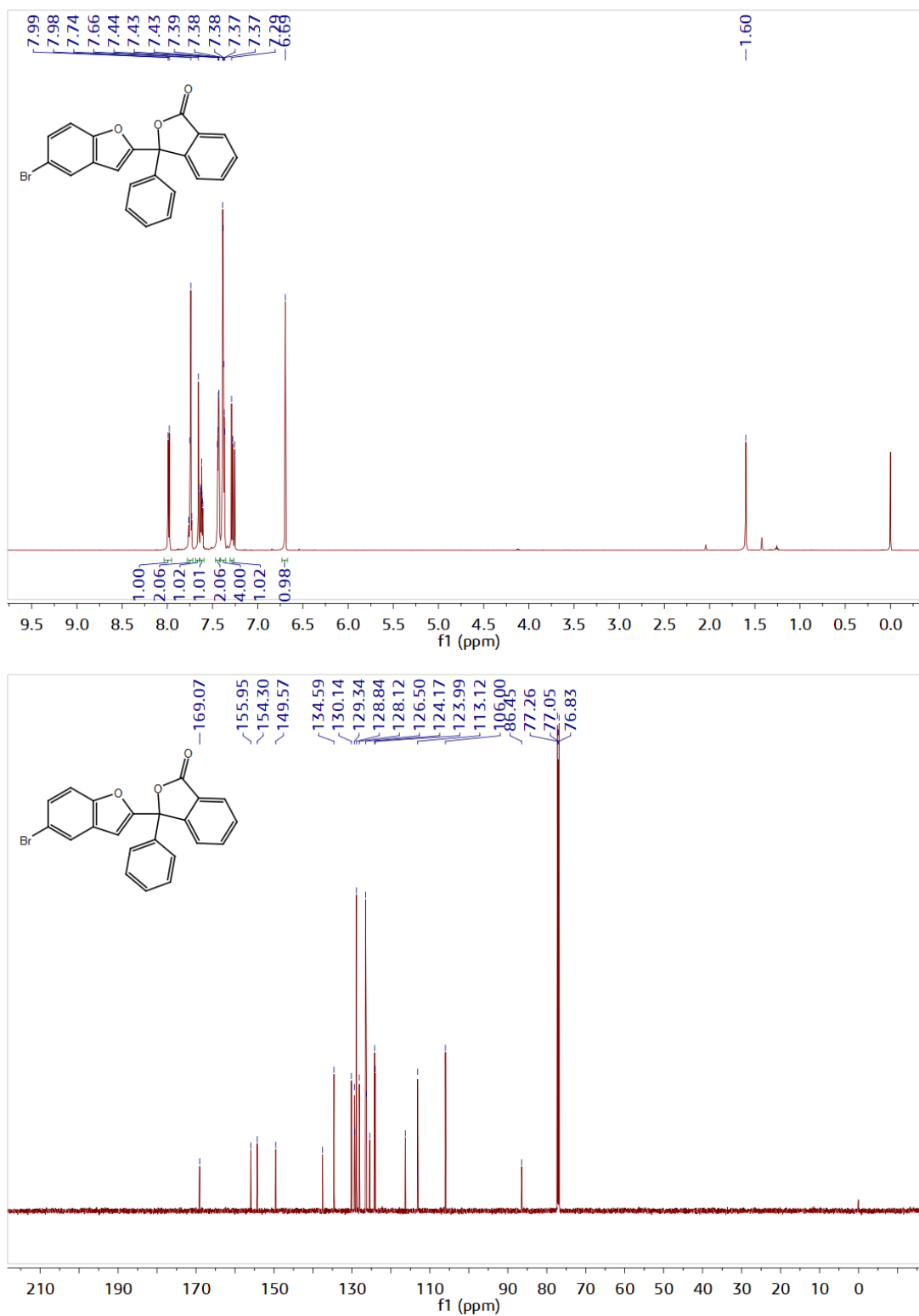
3-(benzofuran-2-yl)-3-phenylisobenzofuran-1(3H)-one (3p). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



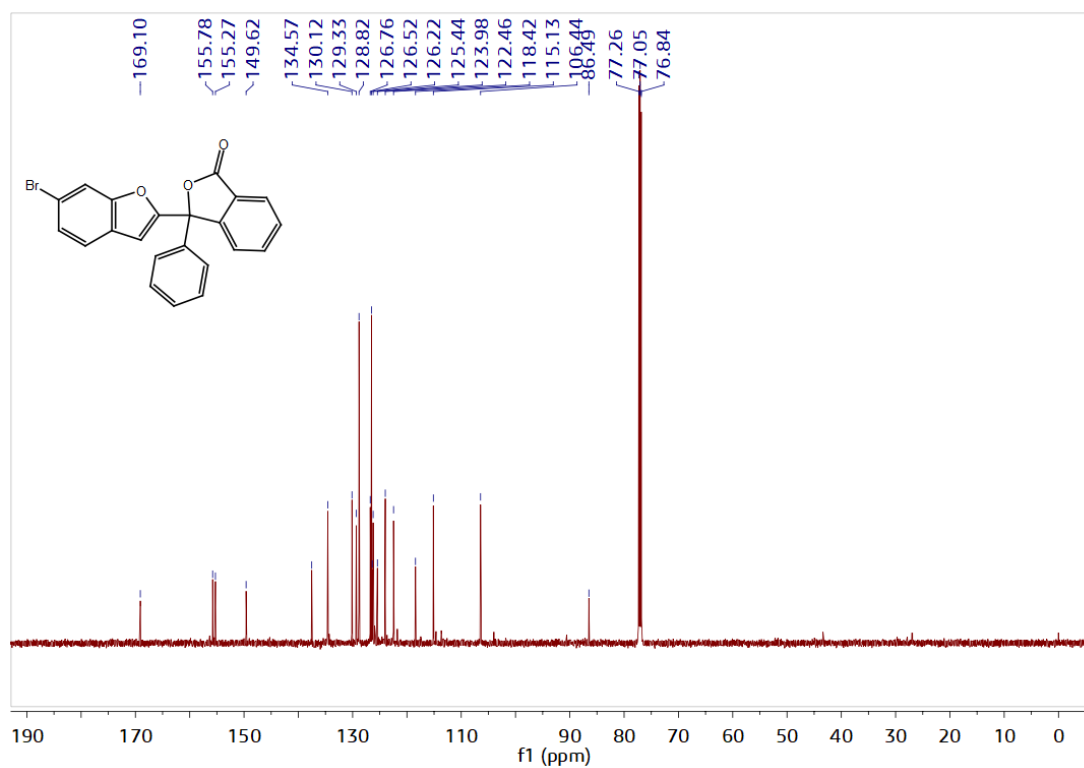
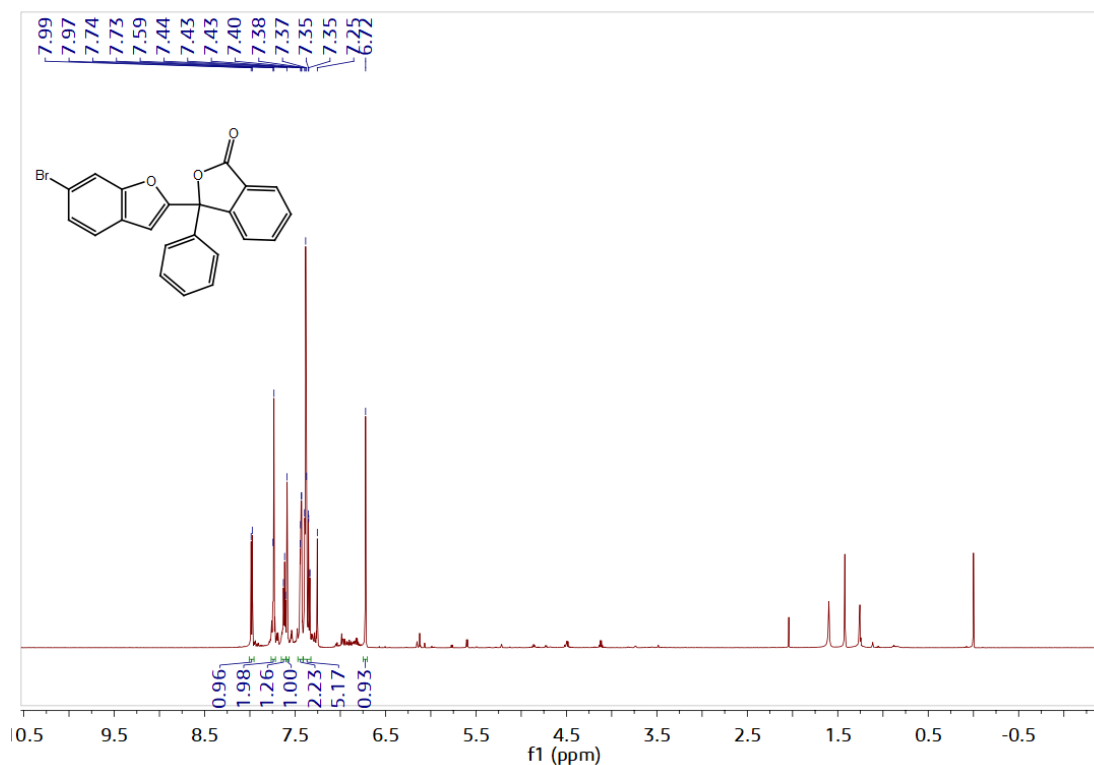
3-(7-bromobenzofuran-2-yl)-3-phenylisobenzofuran-1(3H)-one(3q). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

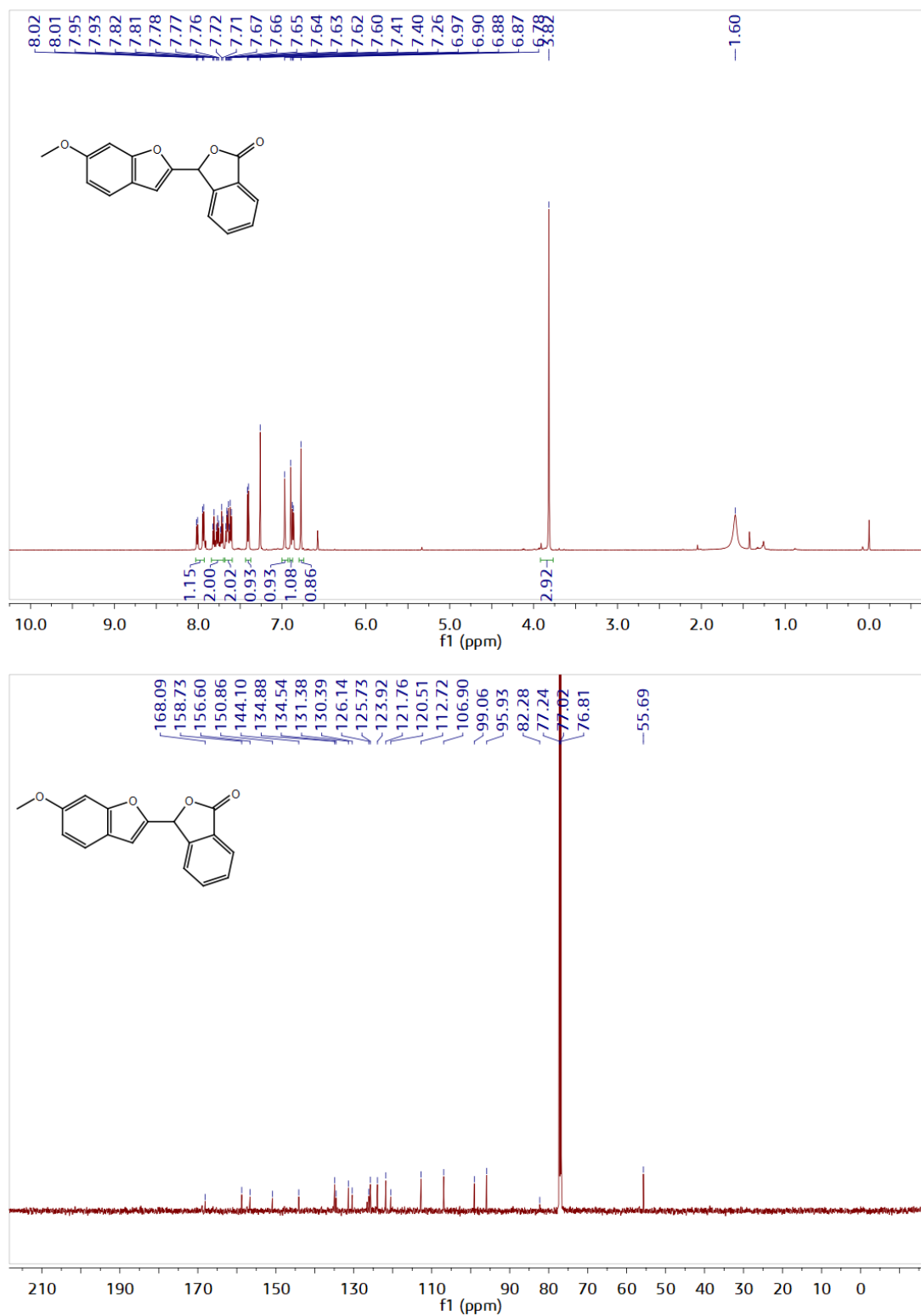


3-(5-bromobenzofuran-2-yl)-3-phenylisobenzofuran-1(3H)-one (3r). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

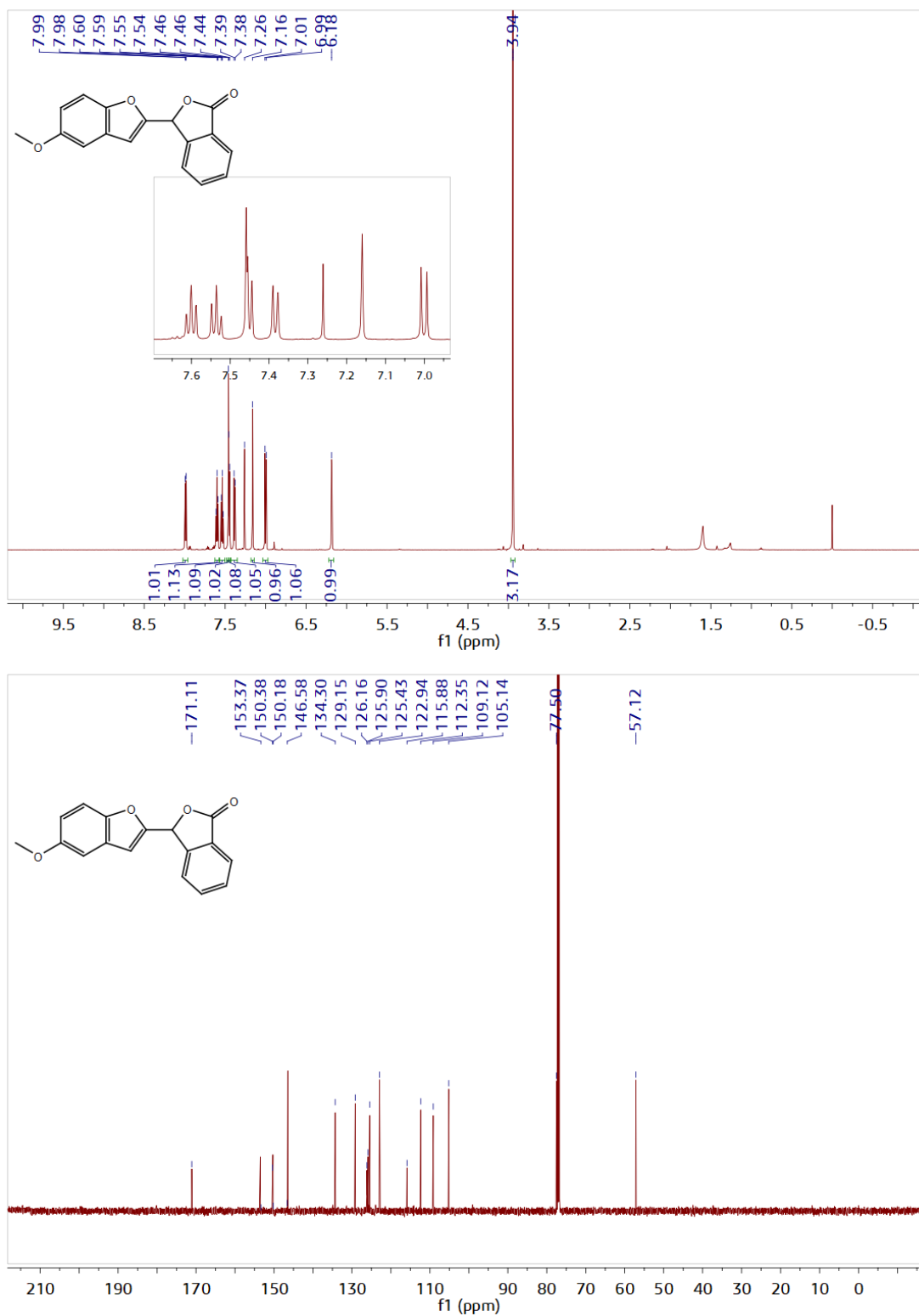


3-(6-bromobenzofuran-2-yl)-3-phenylisobenzofuran-1(3H)-one (3s). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

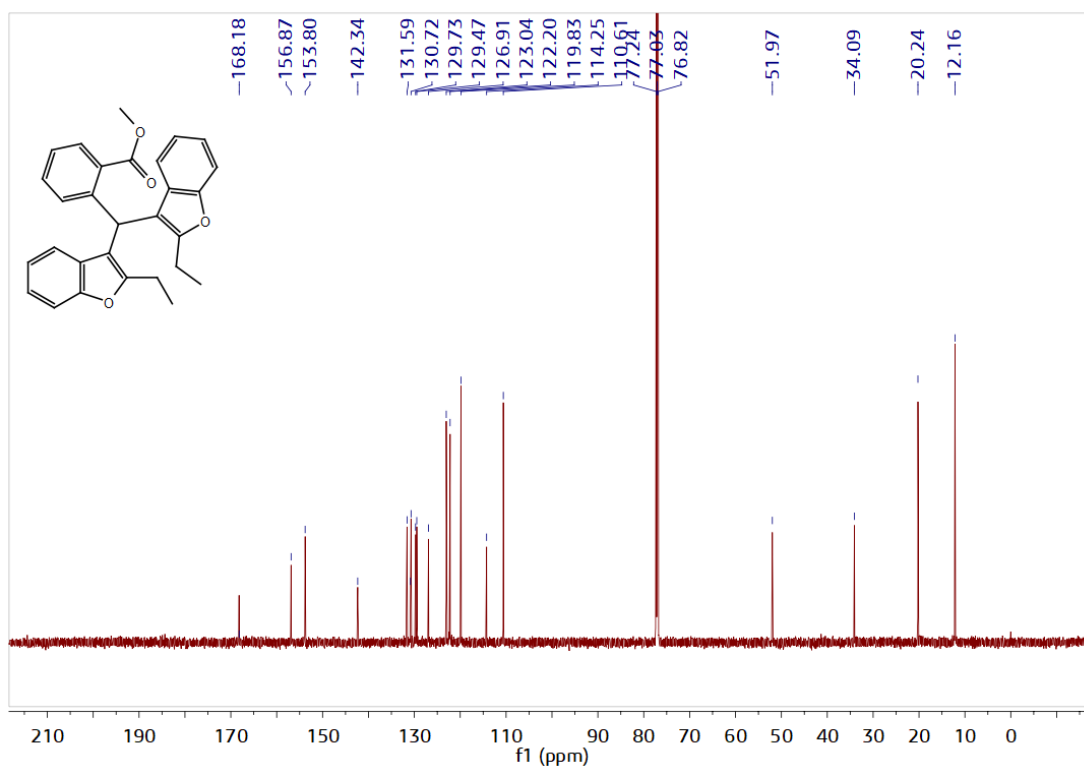
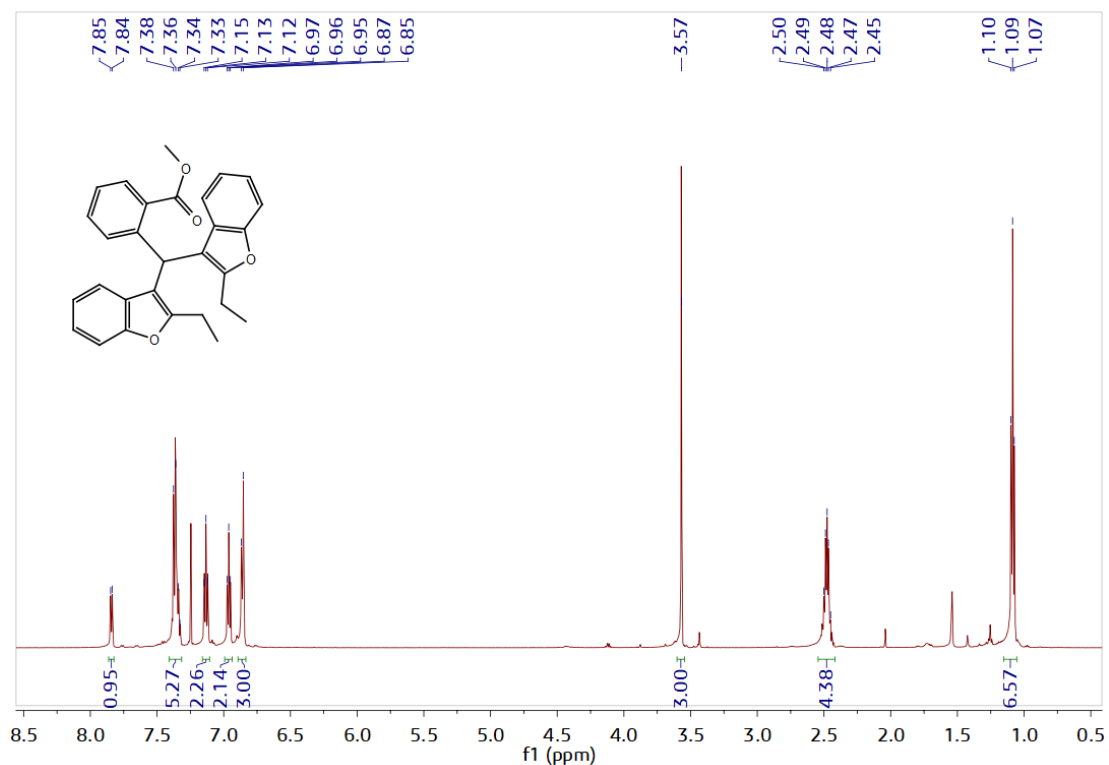


3-(6-methoxybenzofuran-2-yl)isobenzofuran-1(3H)-one (3t). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)

3-(5-methoxybenzofuran-2-yl)isobenzofuran-1(3H)-one (3u). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



methyl 2-(bis(2-ethylbenzofuran-3-yl)methyl)benzoate (3v). ^1H NMR (600 MHz, CDCl_3); ^{13}C NMR (151 MHz, CDCl_3)



2. X-ray crystallographic data for 3e

TableS1. Crystal data and structure refinement for 3e

Identification code	091706_auto
Empirical formula	C ₂₃ H ₁₃ NO ₃
Formula weight	351.34
Temperature/K	293
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	10.1339(2)
b/Å	11.0557(2)
c/Å	15.3882(4)
α/°	90
β/°	95.565(2)
γ/°	90
Volume/Å ³	1715.93(6)
Z	4
ρ _{calc} /cm ³	1.360
μ/mm ⁻¹	0.737
F(000)	728.0
Crystal size/mm ³	0.06 × 0.05 × 0.04
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	8.768 to 136.31
Index ranges	-9 ≤ h ≤ 12, -13 ≤ k ≤ 12, -18 ≤ l ≤ 17
Reflections collected	13602
Independent reflections	3112 [R _{int} = 0.0571, R _{sigma} = 0.0466]
Data/restraints/parameters	3112/0/244
Goodness-of-fit on F ²	1.071
Final R indexes [I ≥ 2σ(I)]	R ₁ = 0.0536, wR ₂ = 0.1285
Final R indexes [all data]	R ₁ = 0.0628, wR ₂ = 0.1376
Largest diff. peak/hole / e Å ⁻³	0.21/-0.35